

FIG. 1(a)

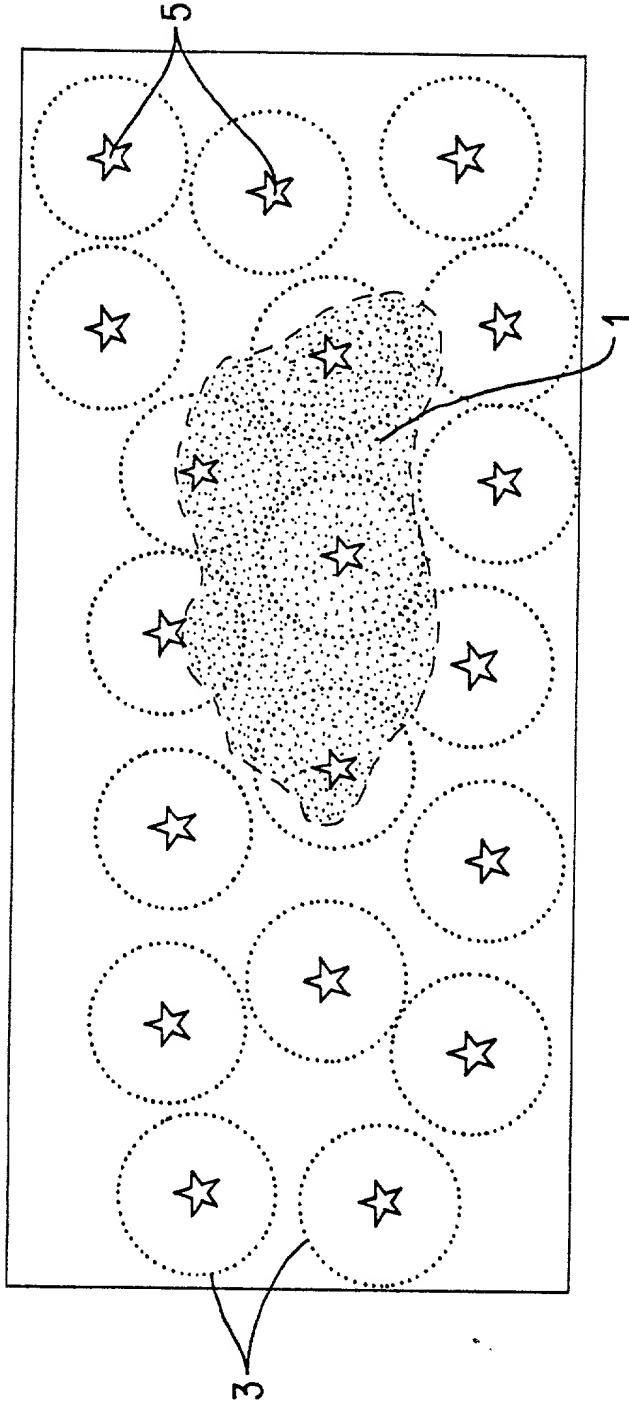


FIG. 1(b)

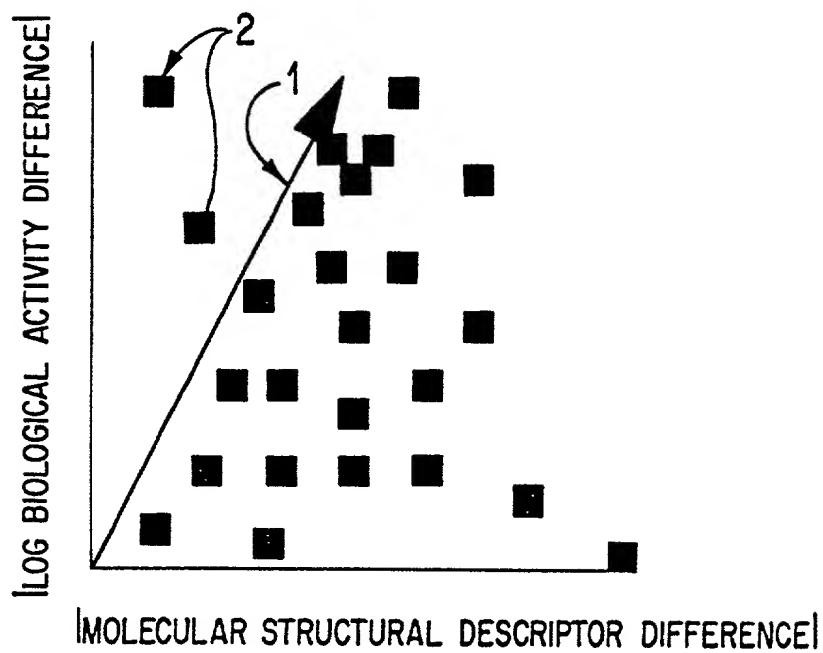


FIG. 2

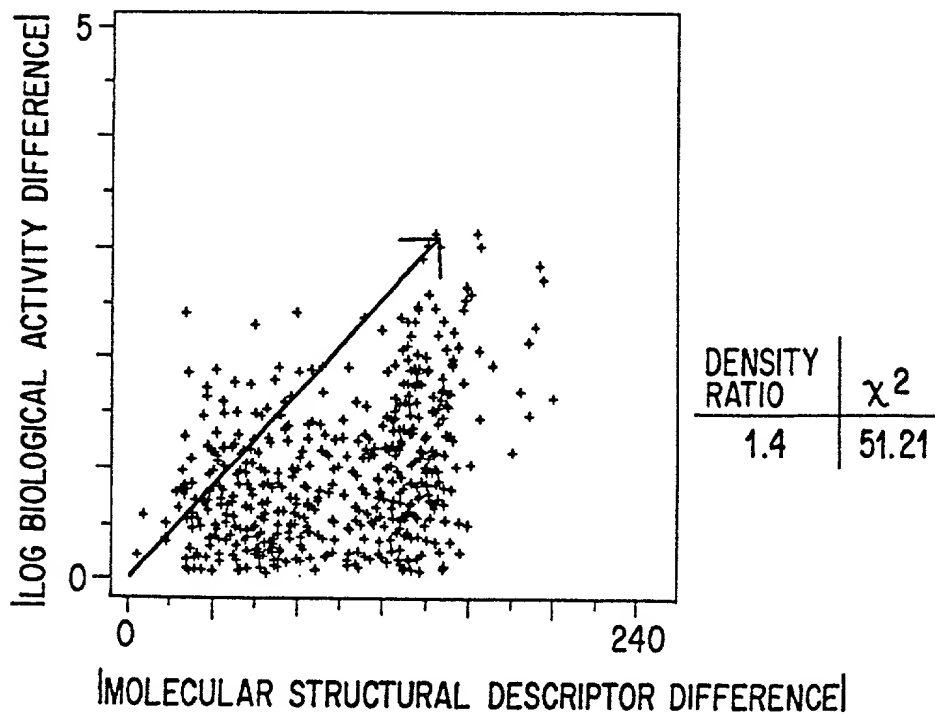


FIG. 3

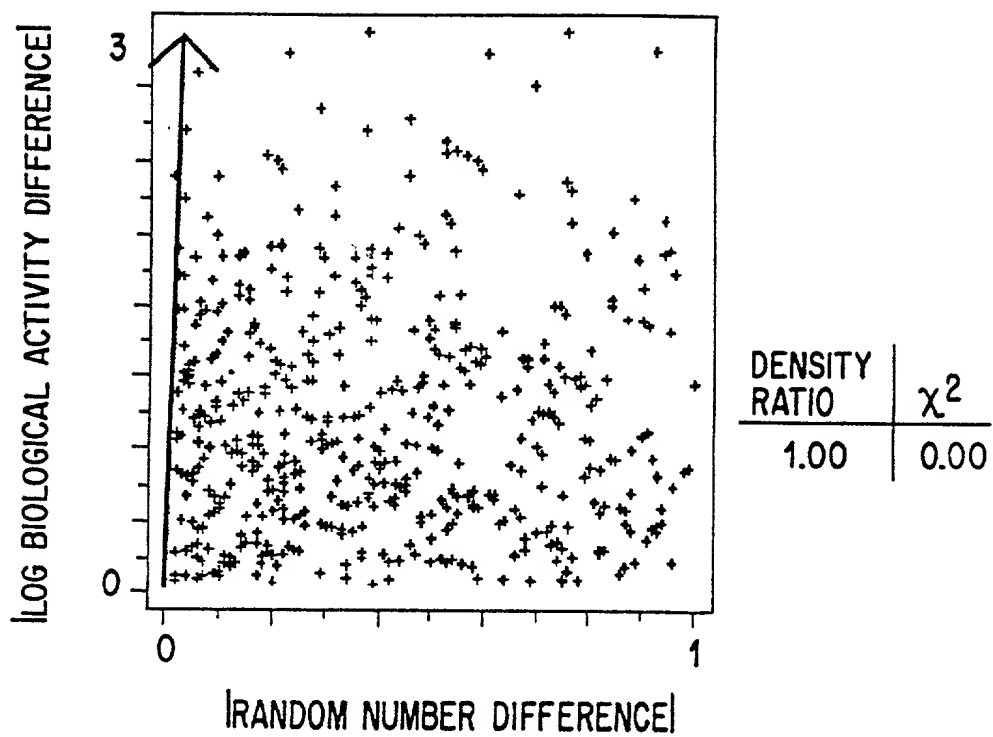


FIG. 4

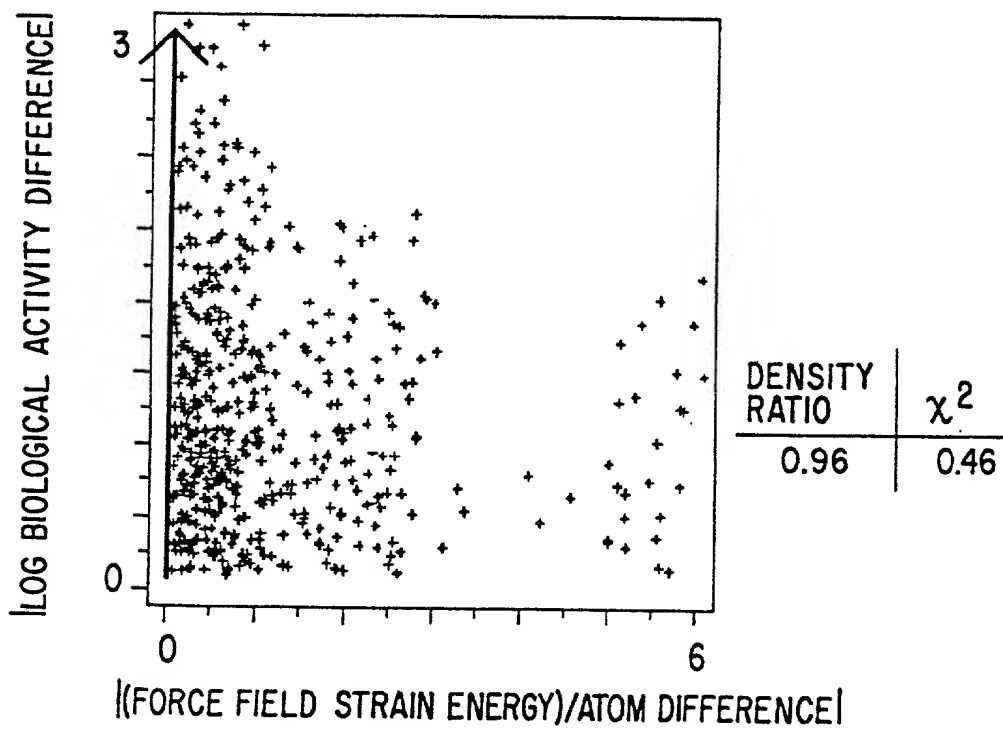
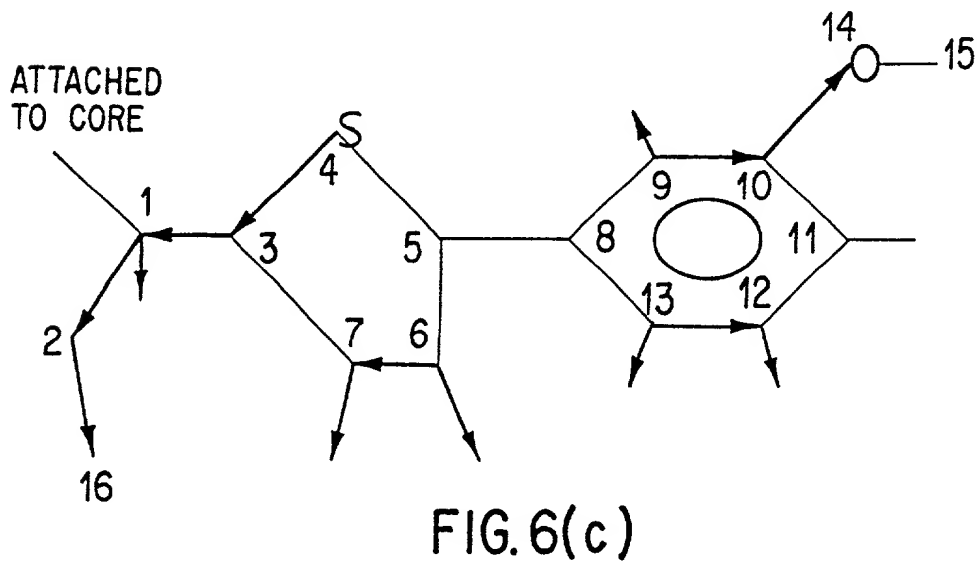
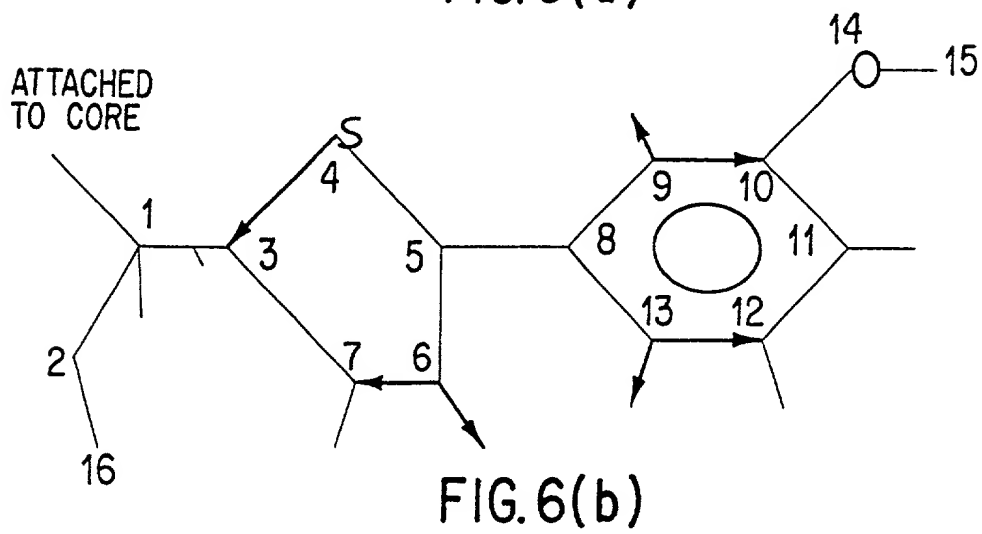
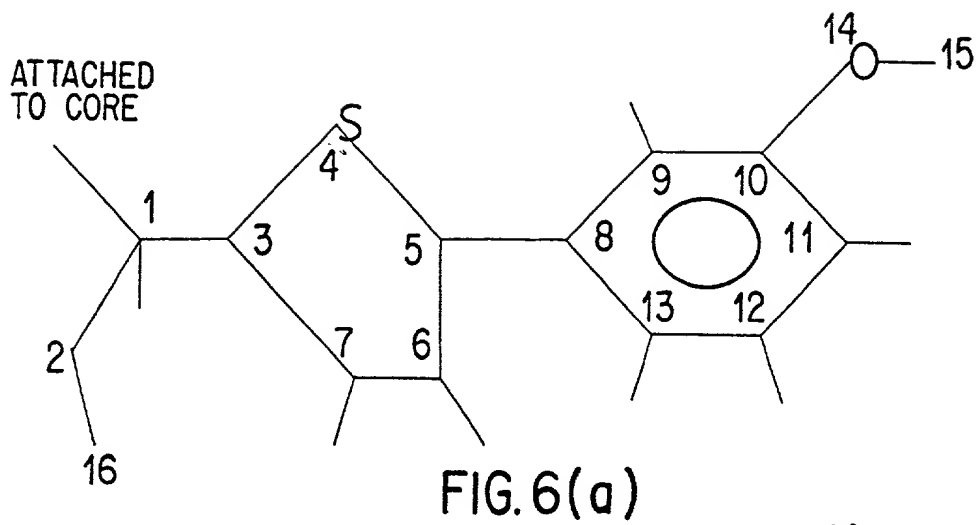


FIG. 5



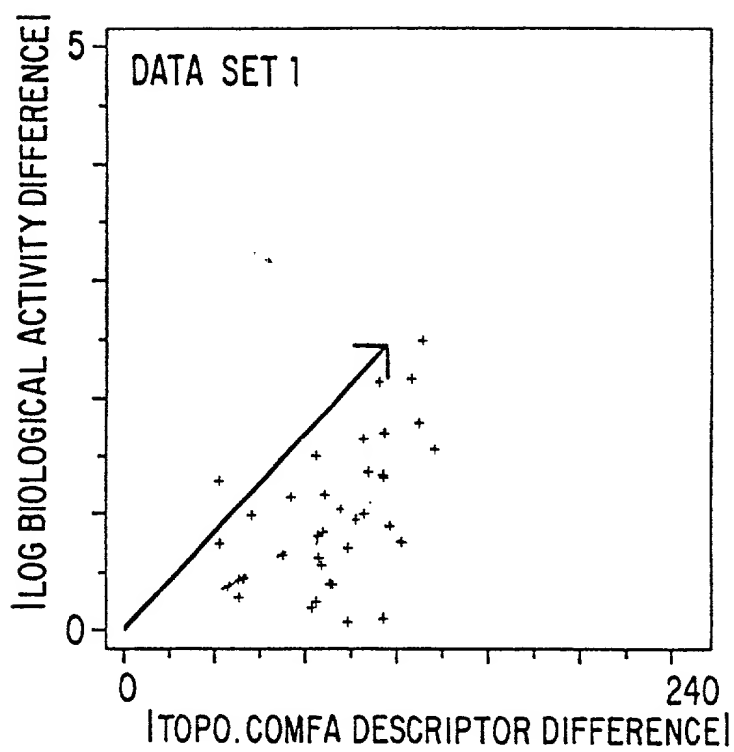


FIG.7(a)

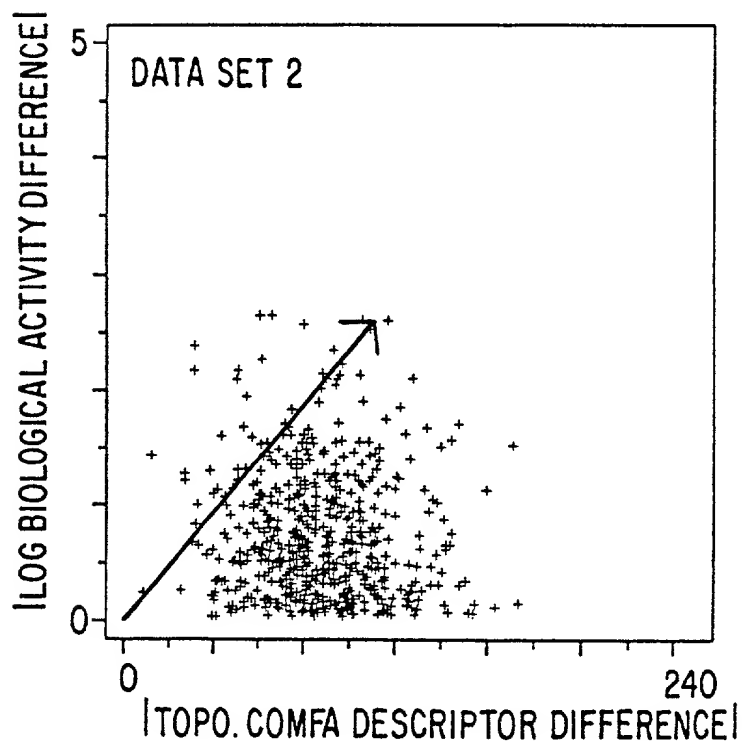


FIG.7(b)

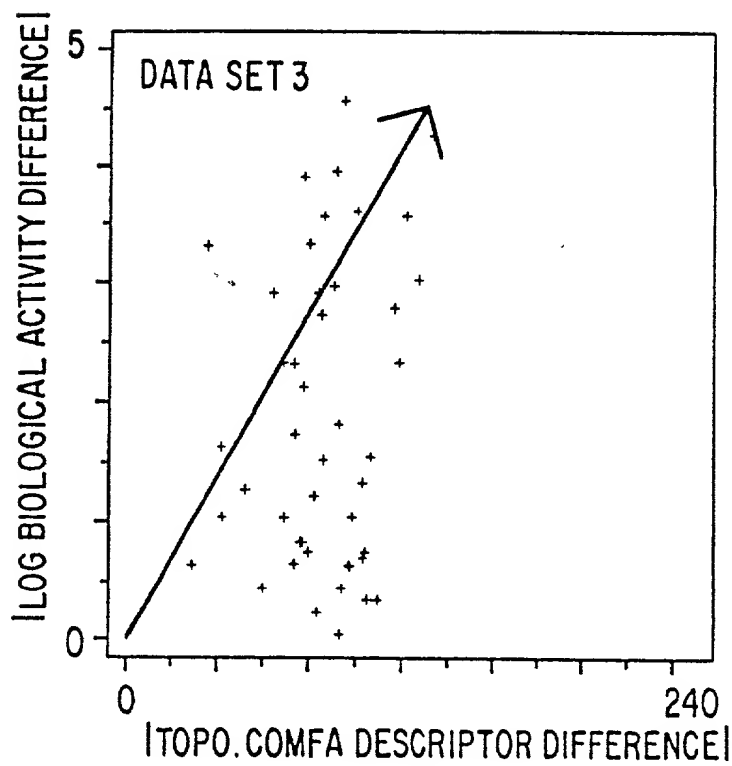


FIG. 7(c)

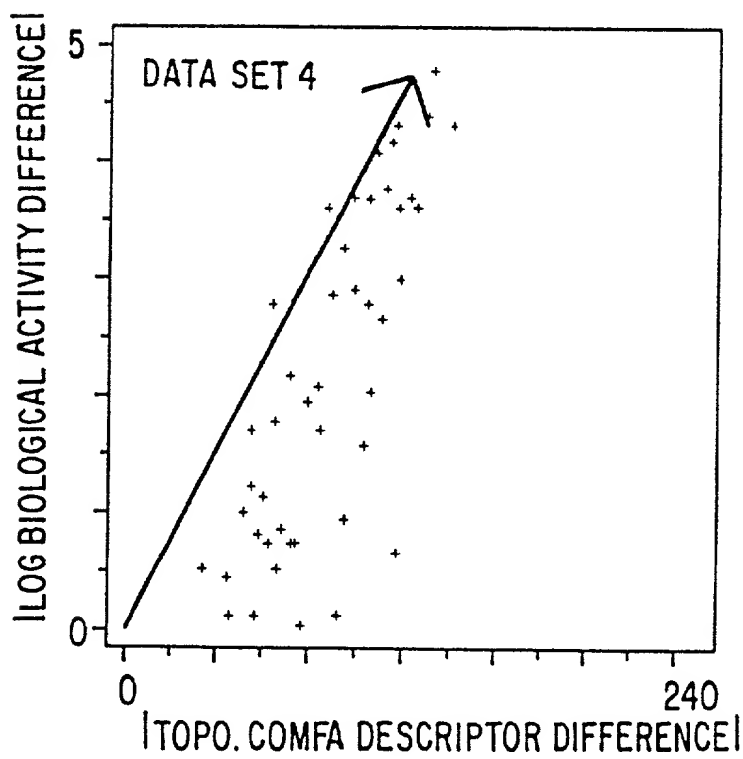


FIG. 7(d)

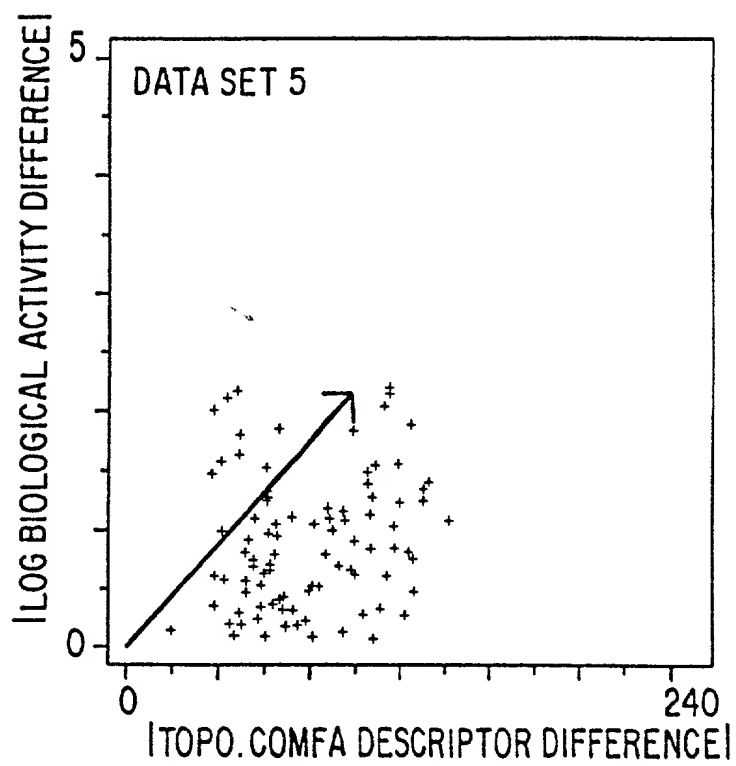


FIG.7(e)

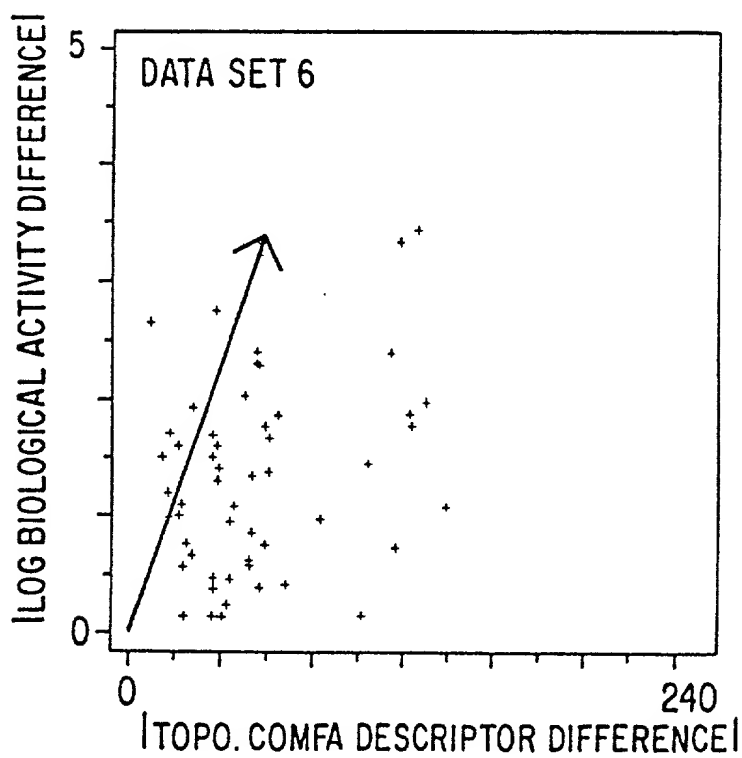


FIG.7(f)

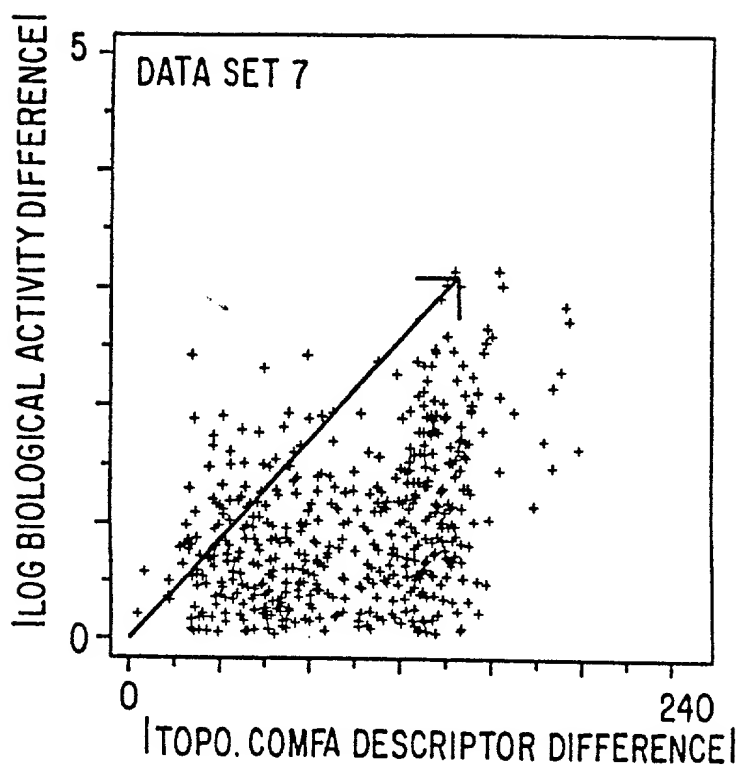


FIG.7(g)

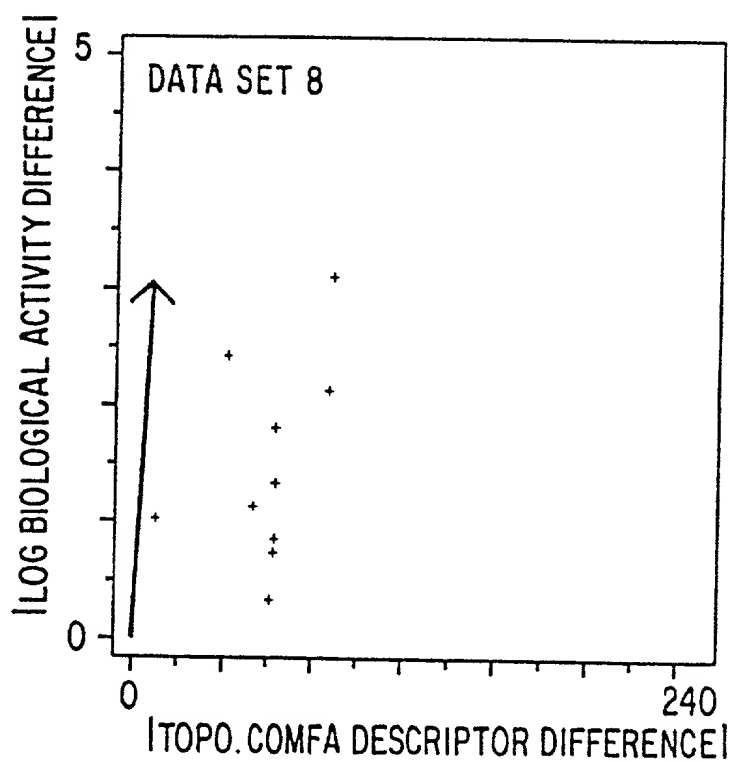


FIG.7(h)

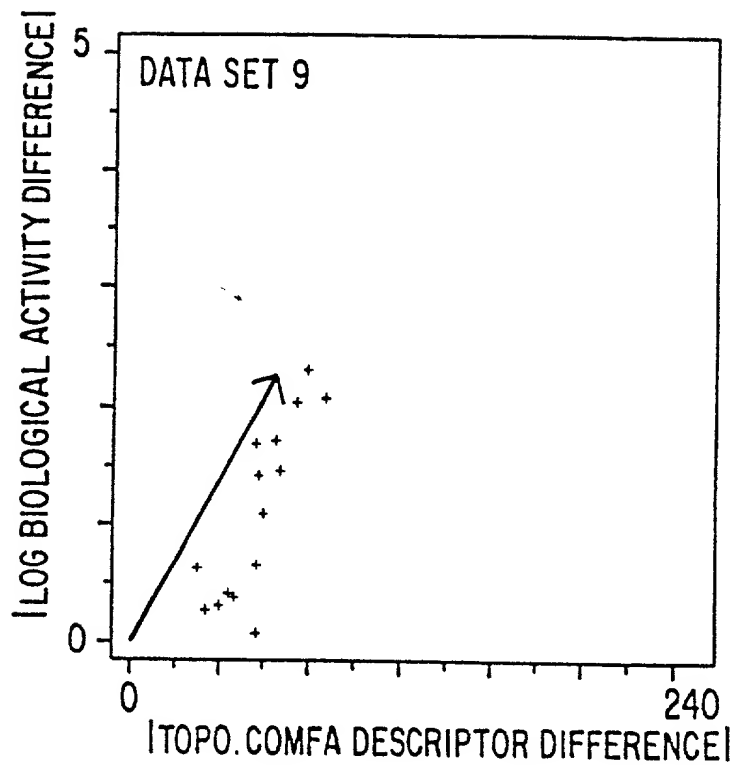


FIG.7(i)

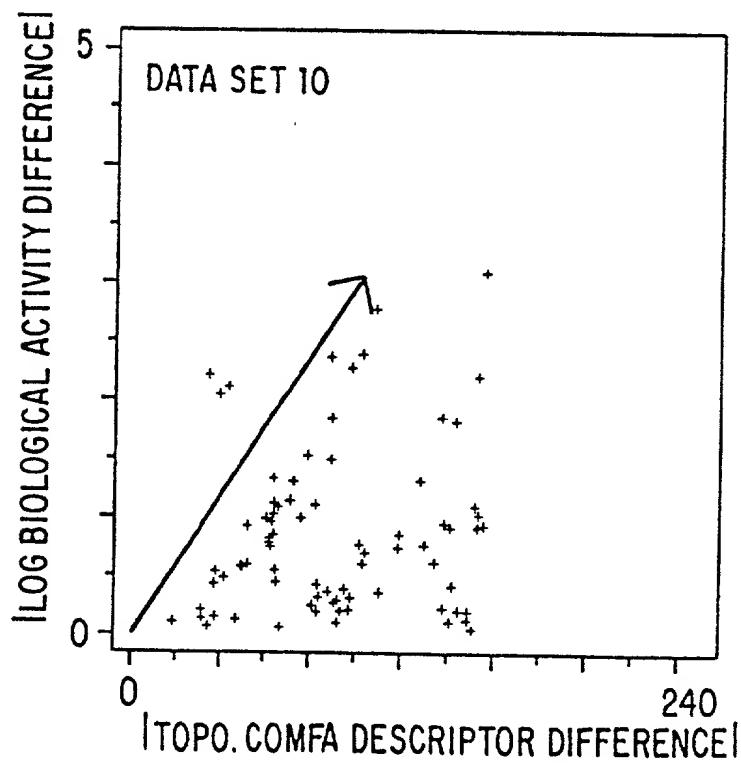


FIG.7(j)

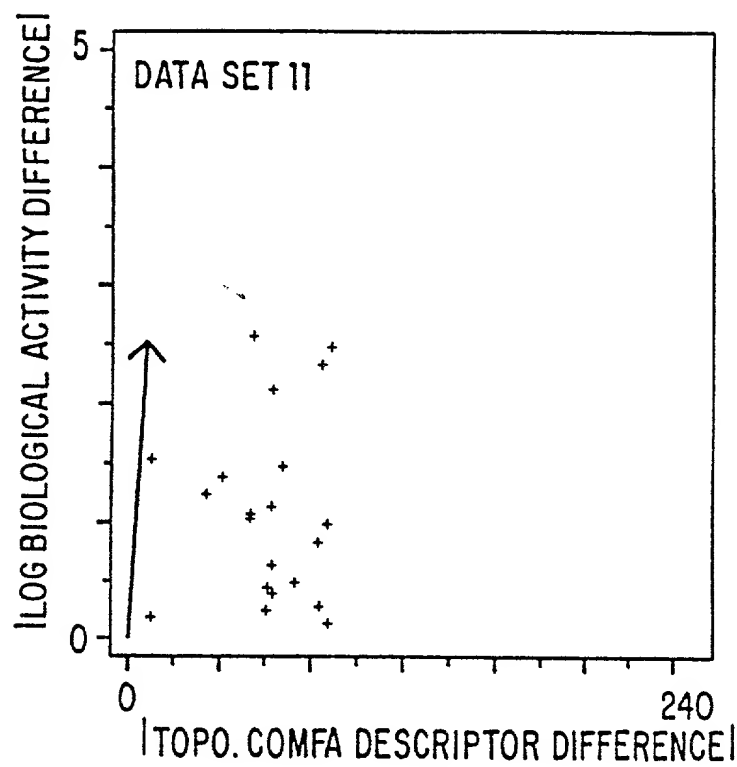


FIG.7(k)

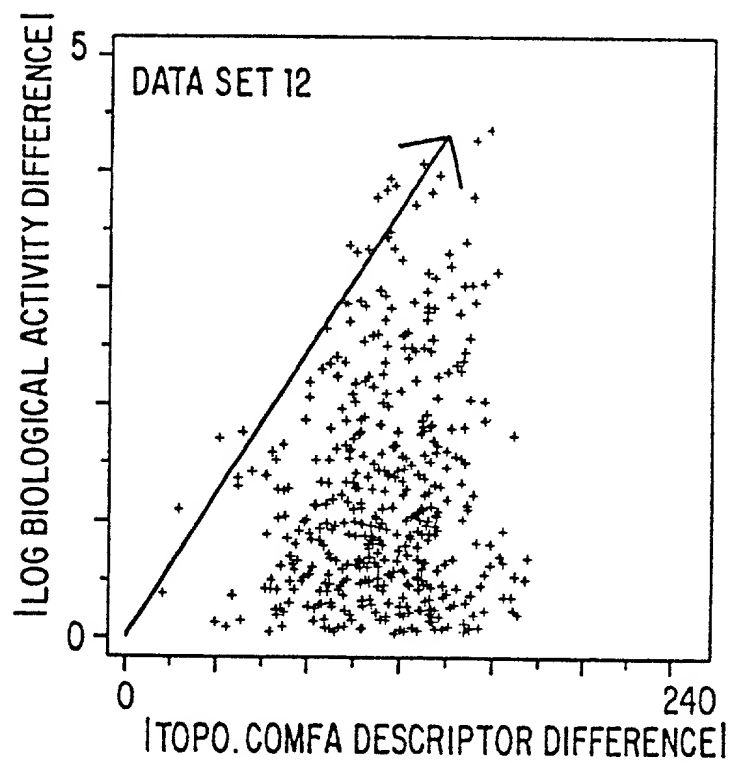


FIG.7(l)

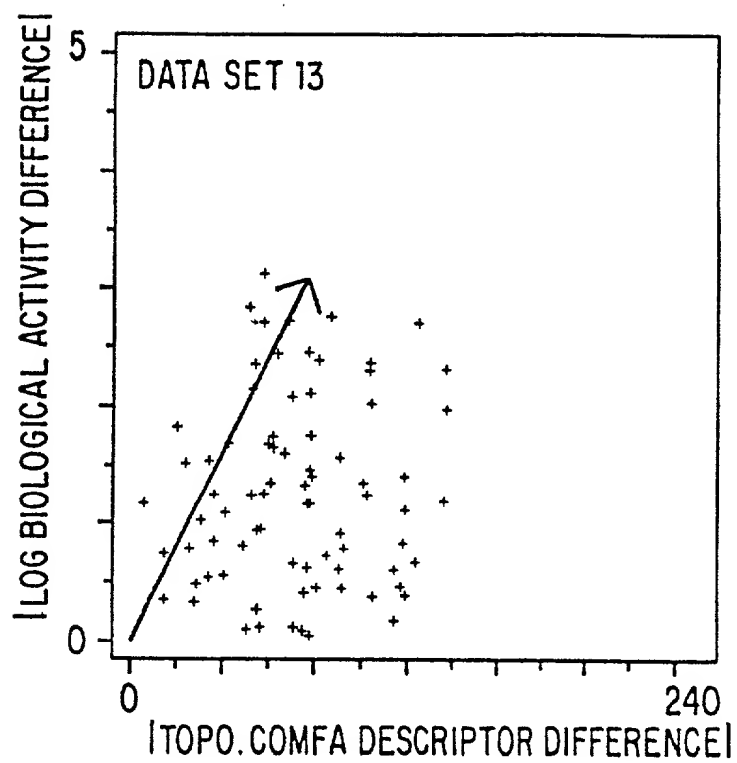


FIG.7(m)

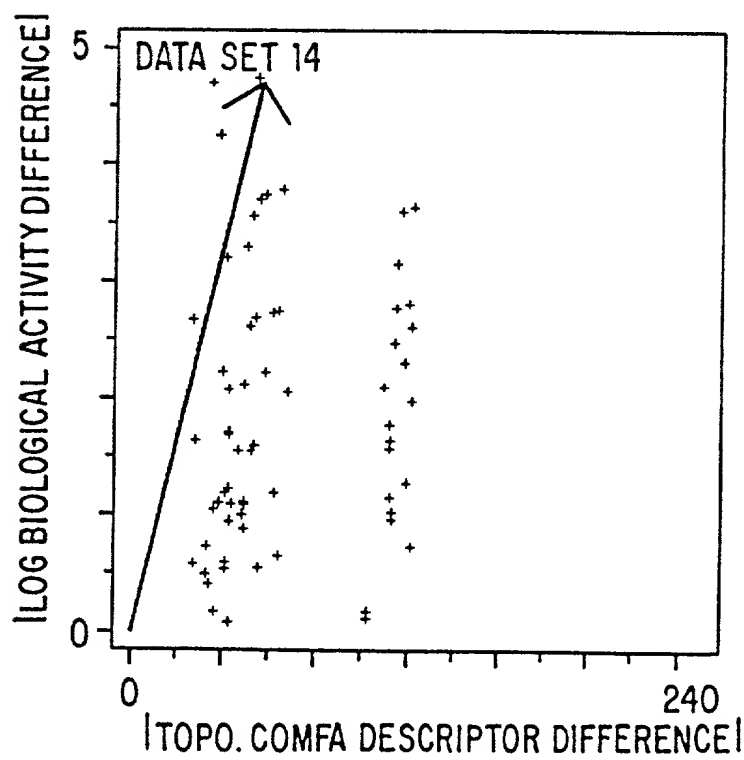


FIG.7(n)

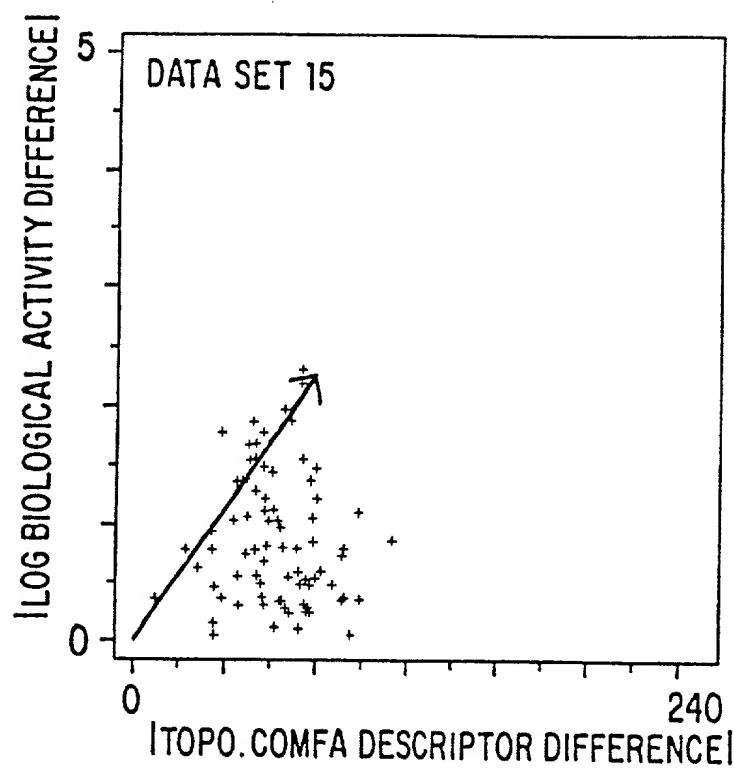


FIG.7(o)

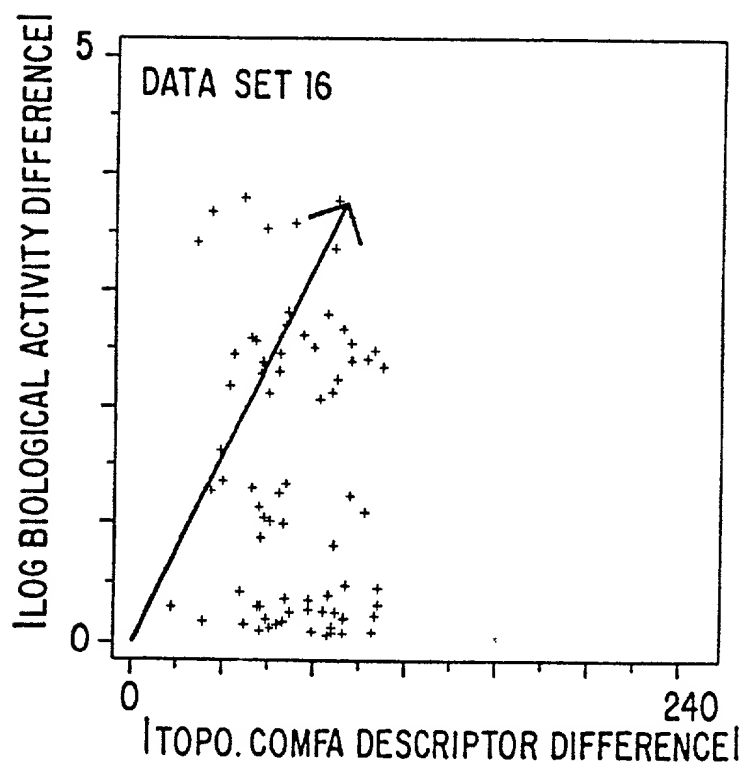


FIG.7(p)

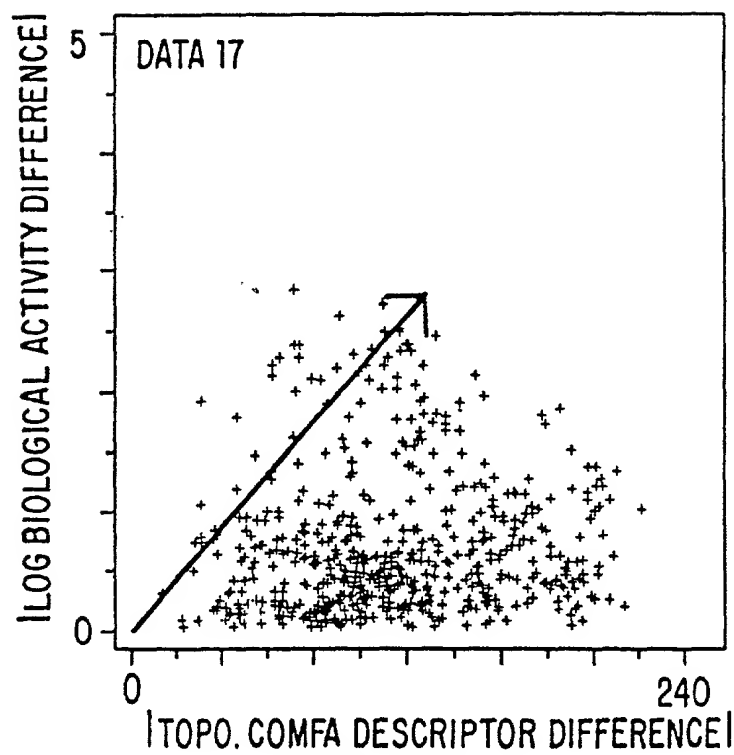


FIG.7(q)

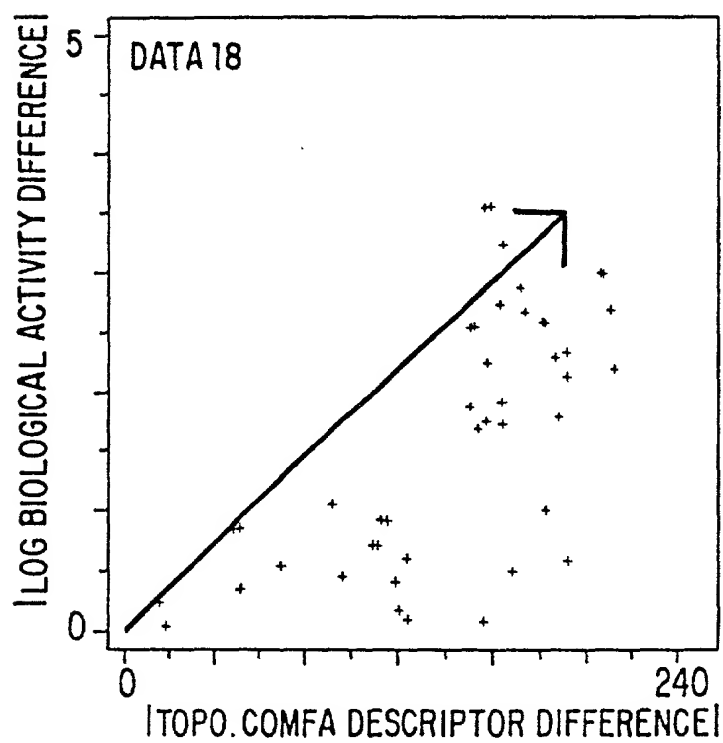


FIG.7(r)

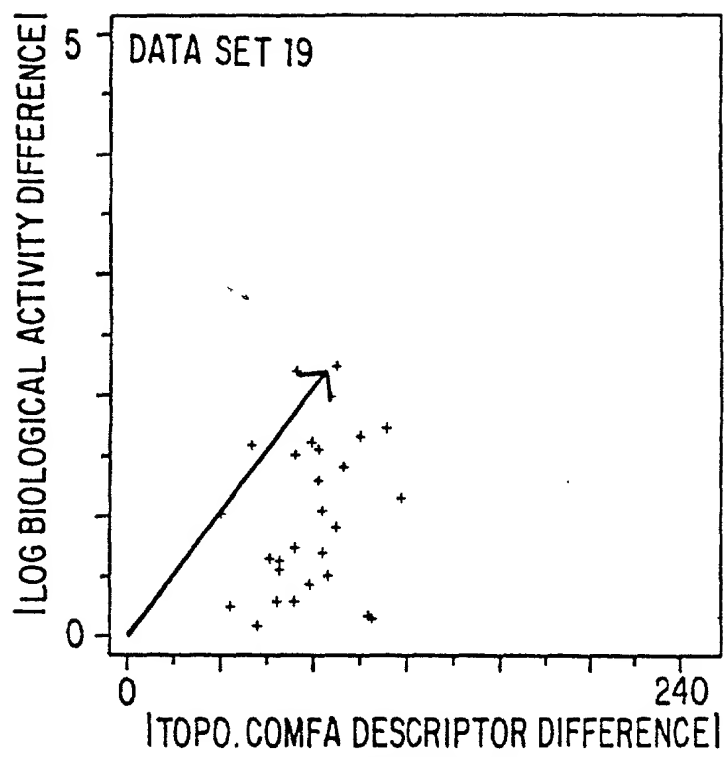


FIG. 7(s)

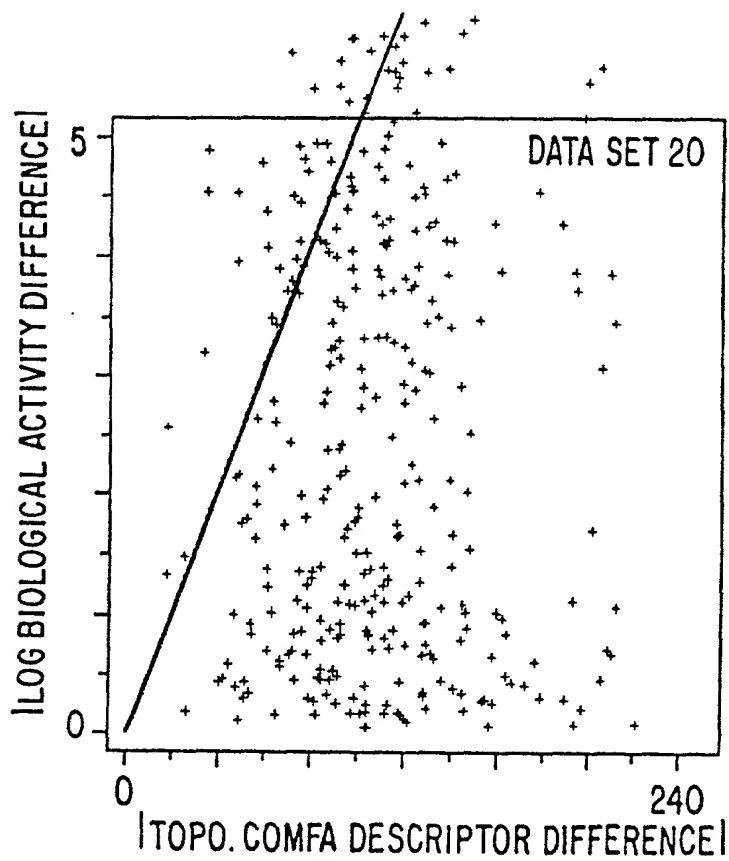


FIG. 7(t)

A scatter plot showing the relationship between CHISO (Y-axis) and RATIO (X-axis). The Y-axis has major ticks at 10 and 140. The X-axis has major ticks at 0.9 and 1.9. The data points, marked with '+', show a general upward trend, with CHISO values increasing as RATIO increases, though there is significant scatter. A few points at higher RATIO values reach CHISO values near 140.

↑
1.1

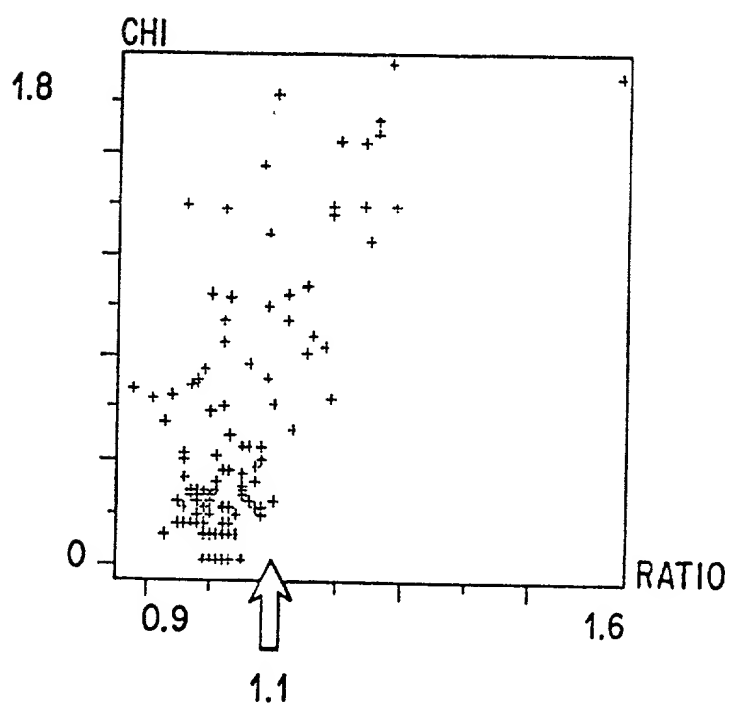


FIG. 8(b)

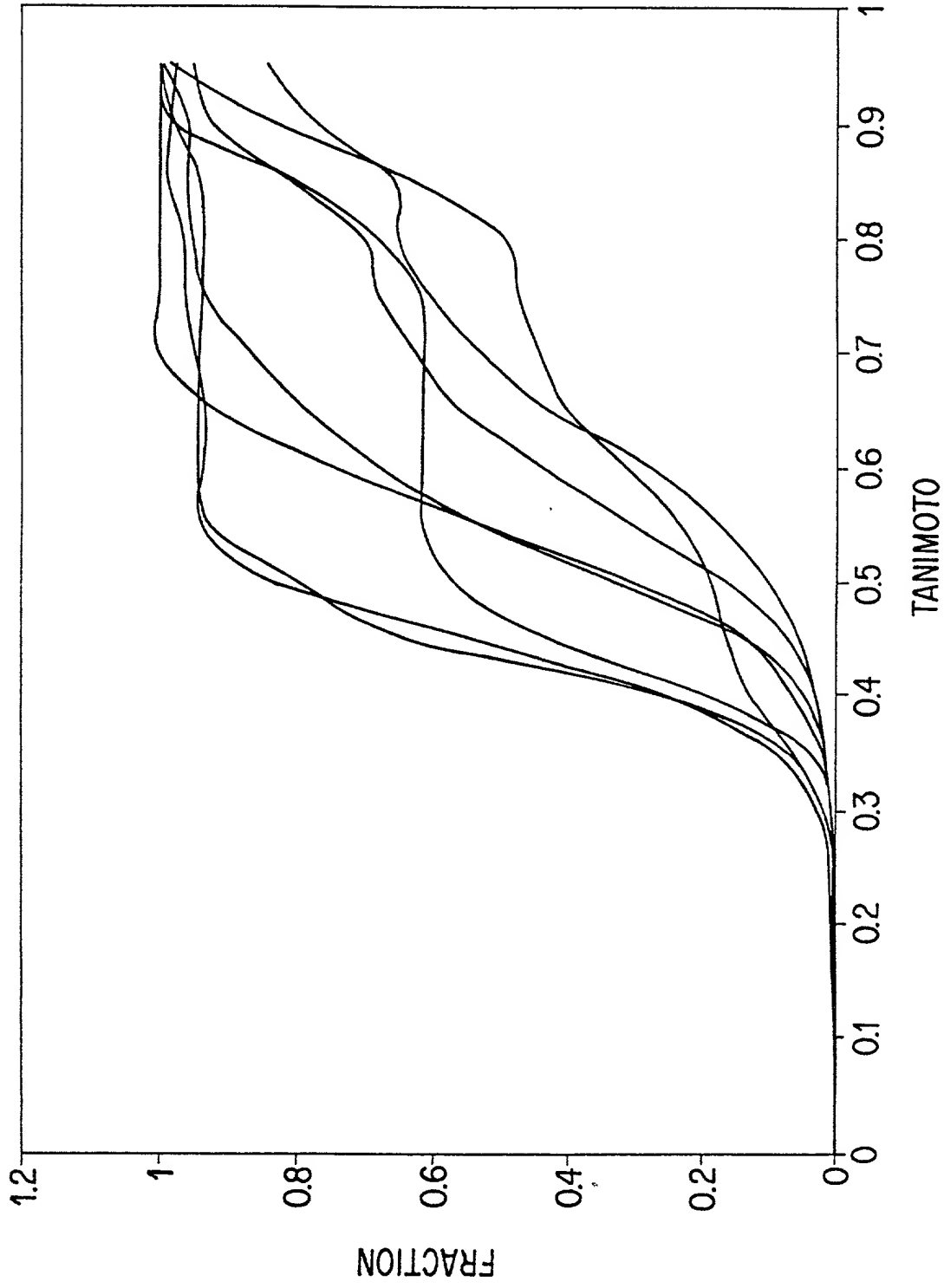


FIG. 9(a)

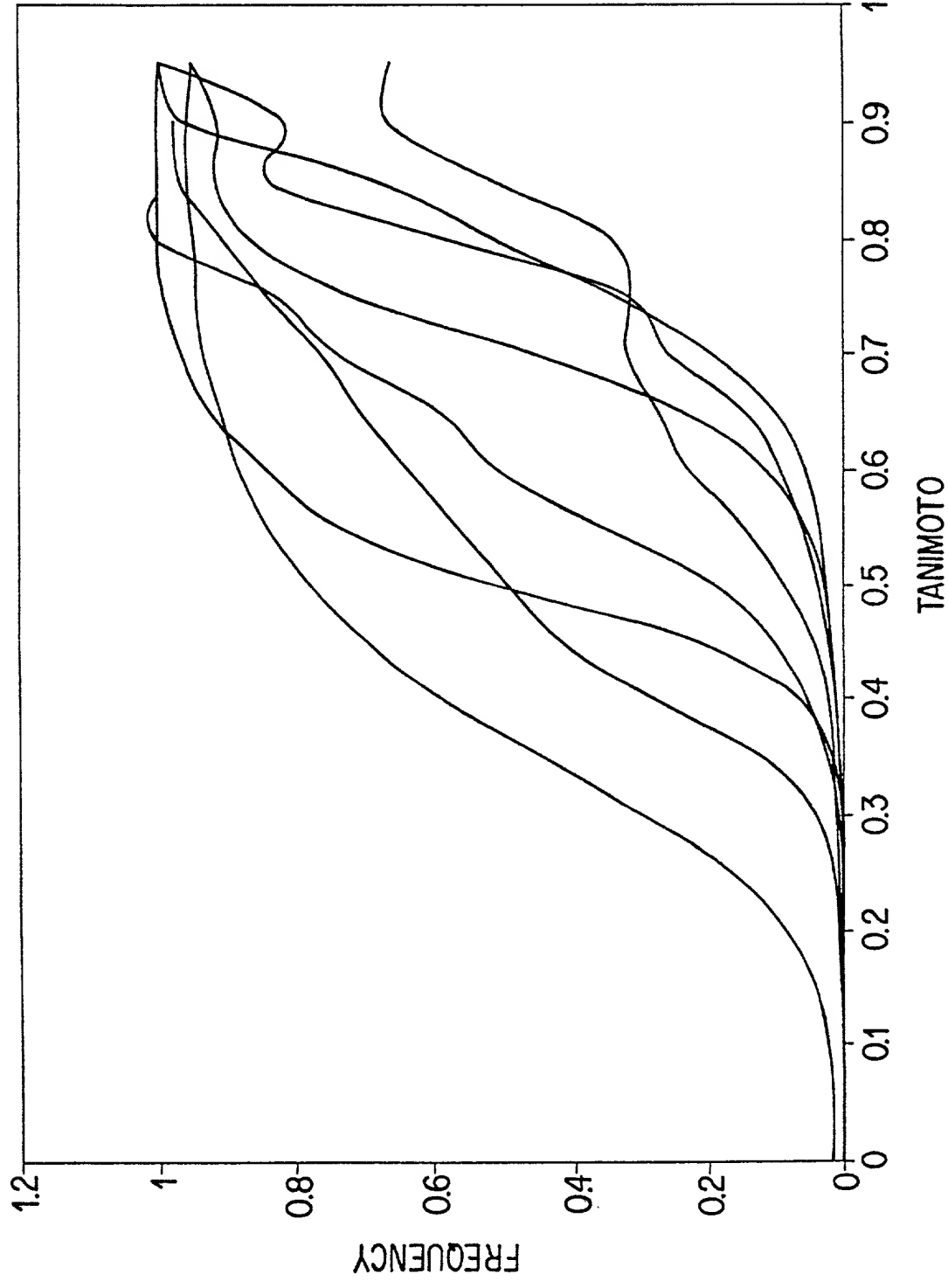


FIG. 9(b)

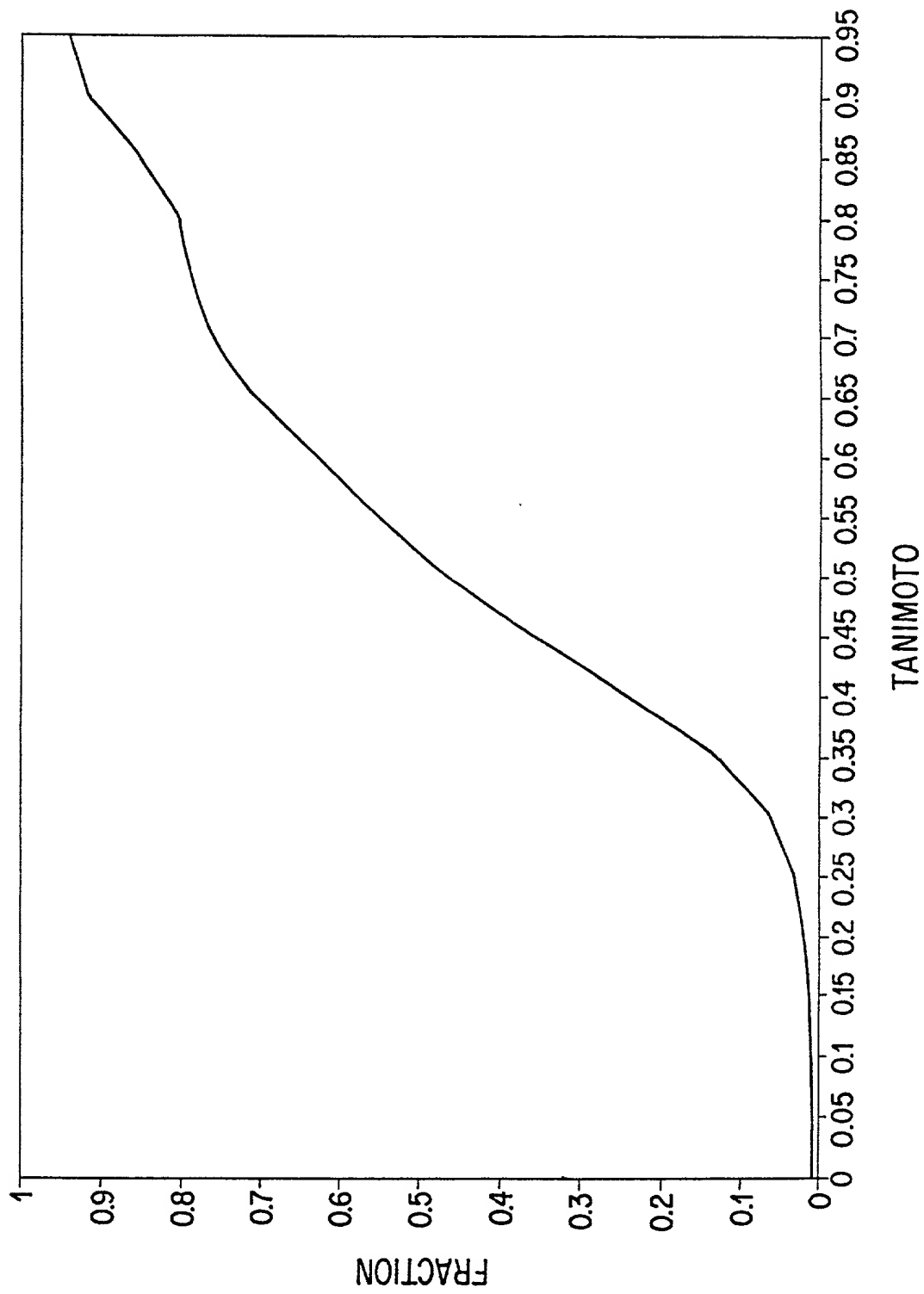


FIG. 9(c)

TOP-300-8025260

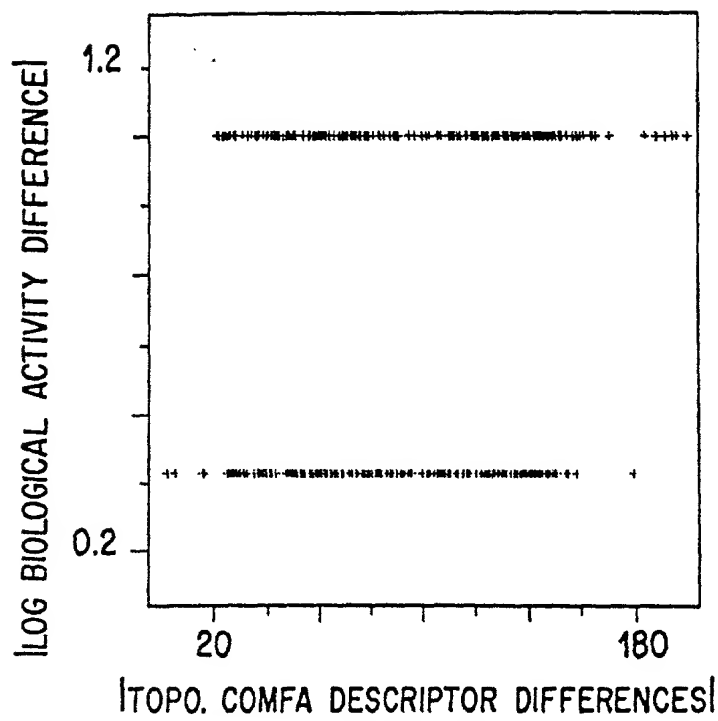


FIG.10(a)

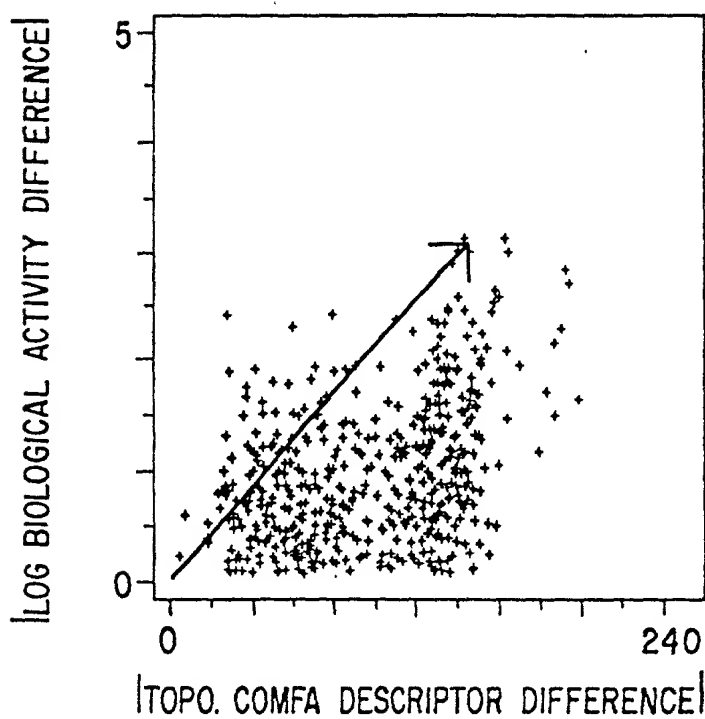


FIG.10(b)

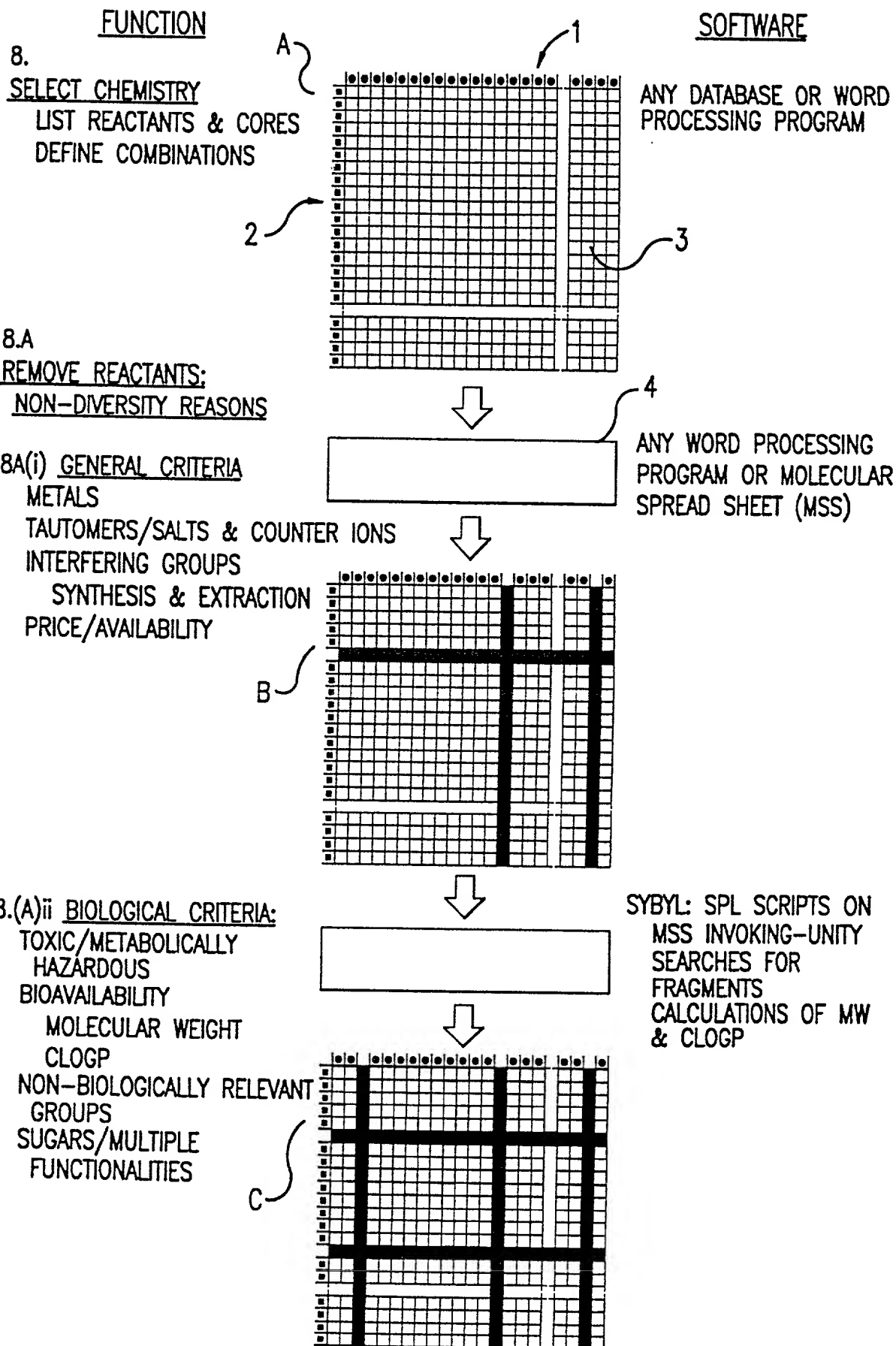
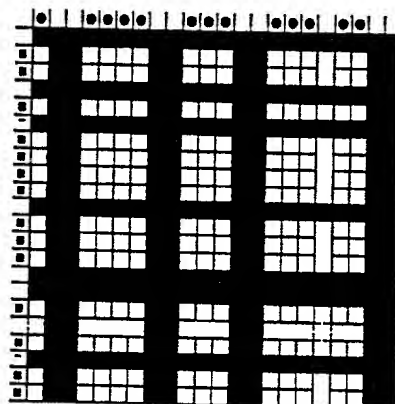
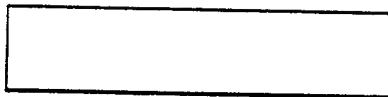


FIG.11(a)

8B

REMOVE NON-DIVERSE REACTANTS:

3D STRUCTURE GENERATION
 TOPOMERIC CONFORMER
 ALIGNMENT
 CoMFA FIELD GENERATION:
 HYDROGEN BOND FIELD
 GENERATION
 ROTATABLE BOND FIELD
 ATTENUATION
 CALCULATE FIELD
 DIFFERENCES
 CLUSTER
 REACTANT SELECTION FROM
 EACH CLUSTER



SYBYL: SELECTOR &
 CONCORD 3.2.1
 SPECIALIZED SOFTWARE:
 APPENDIX "A"
 (SYBYL: CoMFA
 STERIC & MSS)

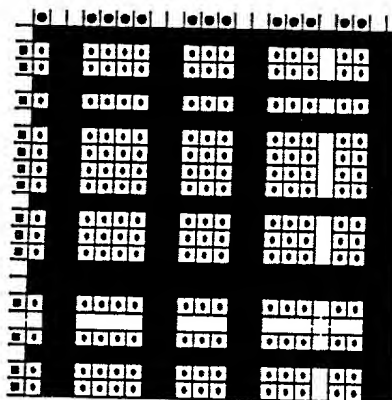
SYBYL: HIERCHICAL
 CLUSTER - MSS
 SYLBL: MSS

8C

COMBINE REACTANTS TO BUILD PRODUCTS



E

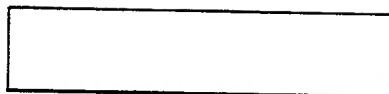


SYBYL: LEGION MSS

8D

REMOVE PRODUCTS:
NON-DIVERSITY REASONS

GENERAL CRITERIA:



SYBYL: SPL SCRIPTS
 ON MSS

F

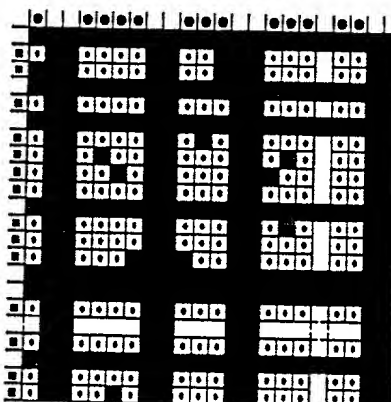


FIG.11(b)

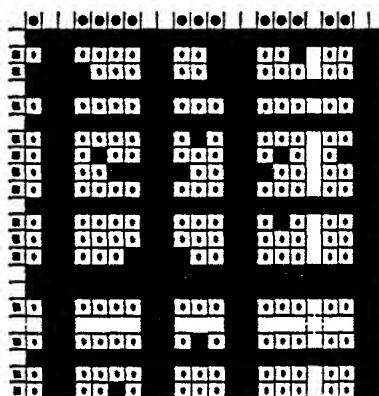
105029-80292260

8D

BIOLOGICAL CRITERIA:
METABOLICALLY HAZARDOUS
BIOAVAILABILITY
MOLECULAR WEIGHT
CLOGP

SYBYL: SPL SCRIPTS ON
MSS INVOKING -
UNITY SEARCHES FOR
FRAGMENTS
CALCULATIONS OF MW
& CLOGP

G



8E

REMOVE NON-DIVERSE
PRODUCTS:

GENERATE TANIMOTO
2D FINGERPRINTS
SAMPLE PRODUCTS:
EXCLUDE TAN ≥ 0.85

UNITY

H

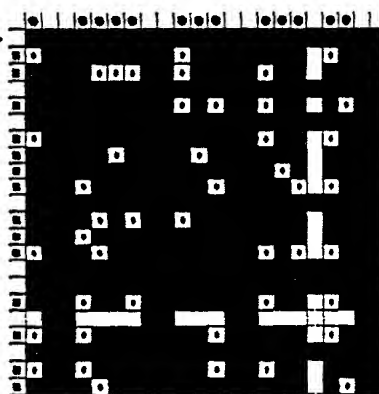


FIG.11(c)

FIG. 12

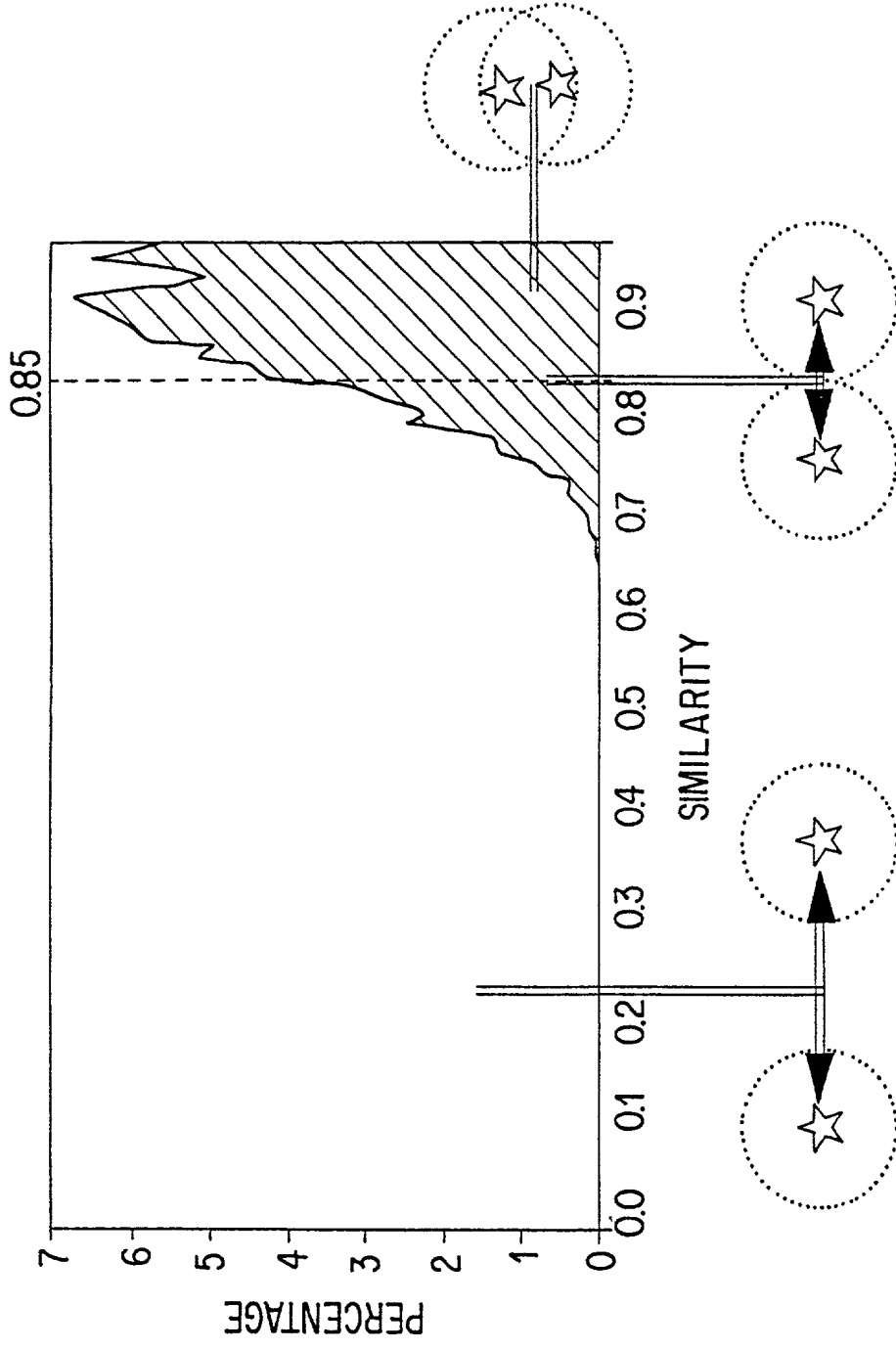


FIG.13

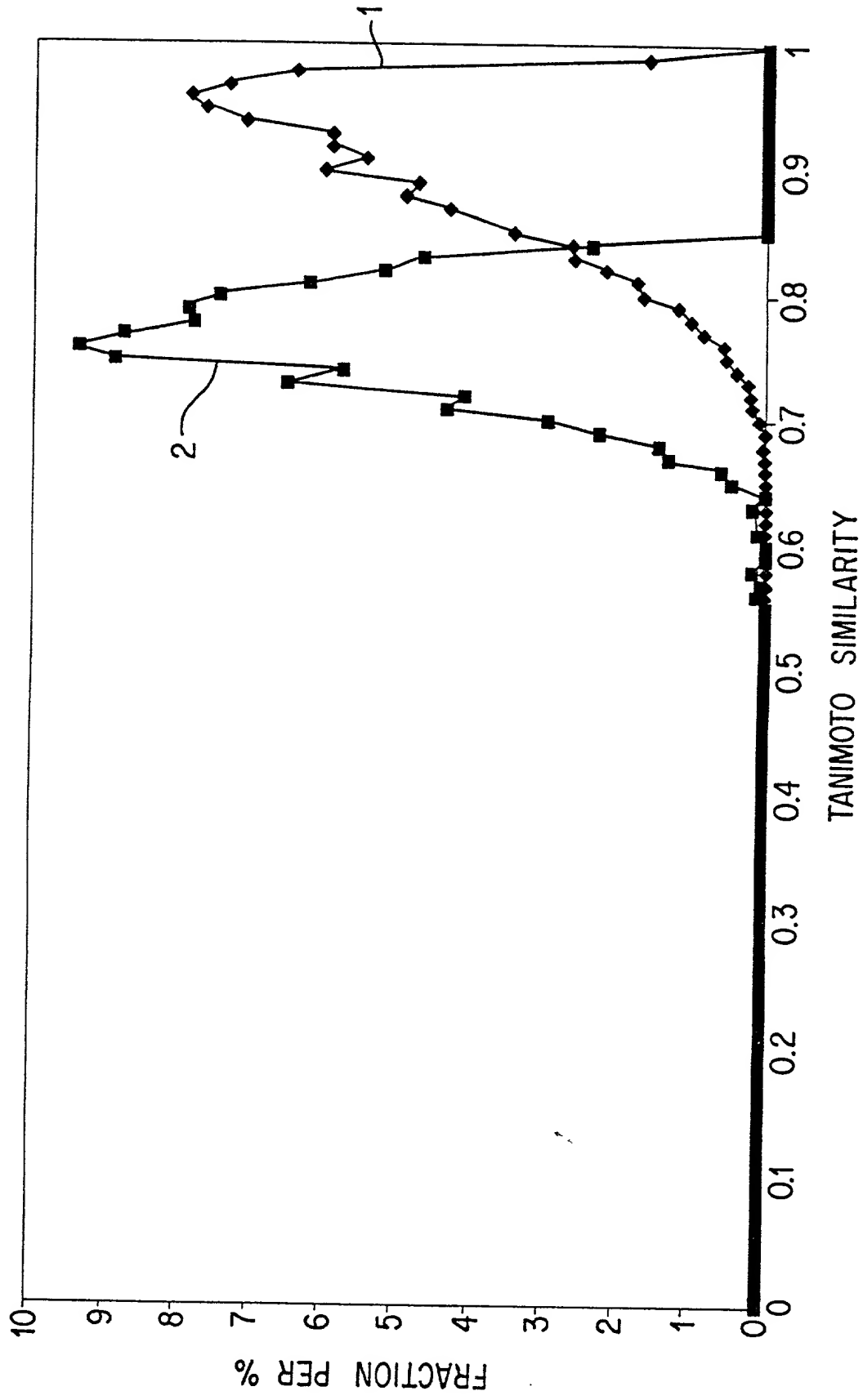


FIG.14

